MONTE CARLO SIMULATIONS IN MEDIA WITH INTERFACES[1]

Antoine Lejay[2]

From joint work with Sylvain Maire[3] and Géraldine Pichot[4]

Diffusion problems in media with interfaces between sub-domains are ubiquitous. Discontinuities in the diffusivity, or thin layers, lead for example to such problems.

We are interested in developing Monte Carlo methods, where a quantity of interest (pressure, concentration, effective coefficient, ...) is computed by using the empirical distribution of a cloud of particles moving independently and randomly in such media. Applications may be found in geophysics, brain imaging, atmospheric study, population ecology, astrophysics, oceanography, chemistry, ...

More precisely, we consider a one-dimensional infinite medium with an interface at 0 separating two parts of constant diffusivity $D(x) = D^-$ for $x < 0$ and $D(x) = D^+$ for $x > 0$. The concentration of a fluid evolving in the media is governed by the Fick's second law

$$\partial_t C(t,x) = \nabla(D(x)\nabla C(t,x)),\ x \neq 0,\ t > 0 \text{ and } C(0,x) = C_0(x). \tag{$\star$}$$

As such, ($\star$) does not define properly the PDE unless one specifies some conditions at 0. There are two kind of interfaces conditions we consider here:

$$\begin{cases} C(t,0-) = C(t,0+), \\ (1-q)D^-\nabla C(t,0-) = (1+q)D^+\nabla C(t,0+) \end{cases} \tag{$\mathcal{I}1$}$$

for some $q \in (-1,1)$ and

$$\begin{cases} D^+ = D^-, \\ \nabla C(t,0-) = \nabla C(t,0+), \\ \lambda(C(t,0+) - C(t,0-)) = D^\pm \nabla C(t,0\pm). \end{cases} \tag{$\mathcal{I}2$}$$

With $q = 0$ in condition ($\mathcal{I}1$), it is a rewriting of ($\star$) on $\mathbb{R}$ with the divergence form operator $\nabla(D\nabla\cdot)$, where this equation is interpreted as a diffraction problem

[1]This conference proceedings has been published in the Oberwolfach Report 41/2013 following the conference *Interplay of Theory and Numerics for Deterministic and Stochastic Homogenization* organized by G. Bal, B. Engquist, C. Le Bris and H. Owhadi at the Mathematisches Forschungsinstitut Oberwolfach, Germany, in March 2013.

[2]Université de Lorraine, IECL, Nancy, F-54506, France / CNRS, IECL, Nancy, F-54506 / Inria, Vilers-lès-Nancy, F-54600, France

[3]Université de Toulon et du Var

[4]Inria Rennes

(See *e.g.* [3]). With $q = (D(0-) - D(0+))/(D(0+) + D(0-))$, then it corresponds indeed in solving $\partial_t C(t,x) = D(x)\nabla C(t,x)$ over the whole domain. In general, this interface condition can be reached as the limit by homogenization of a process with constant diffusivity and a drift periodic on each side of the interface [2].

Condition ($\mathcal{I}2$) is obtained as the limit of a thin layer problem, that is when the diffusivity is equal to $\epsilon\lambda$ on the layer of width ϵ around 0 decreases to 0 (See *e.g.* [9]).

Monte Carlo simulations. We are looking at simulating particles starting from x whose positions at time t have for density the fundamental solution $p(t,x,\cdot)$ of the problem ($\star$), with respect to the x variable, with the appropriate interface condition.

The successive positions of the particles $t \mapsto X_t$ form continuous but irregular paths. We then aim at simulating a discretized version $(X_0, X_{\delta t}, X_{2\delta t}, \dots, X_T)$ of $(X_t)_{t\in[0,T]}$ for a small time step δt.

For both interfaces conditions, X is a (strong) Markov process so that the distribution of $X_{(k+1)\delta t}$ given $(X_0, \dots, X_{k\delta t})$ depends only on $X_{k\delta t}$. However, X is not in general solution to a Stochastic Differential Equation (SDE).

Here, we are interested in the behavior of the particle at the interface. Our results are easily generalized when D varies smoothly away from 0, in presence of several interfaces or boundary conditions. This is why we take D piecewise constant for the sake of simplicity.

Until it reaches the interface, the particle moves like a Brownian motion of diffusivity $2D^{\pm}$. Thus, the successive positions of the particles are easily simulated by $X_{(k+1)\delta t} = X_{k\delta t} + \sqrt{2D(X_{k\delta t})\delta t} \times \xi$ where ξ is a centered, unit, Gaussian random variable independent from $X_{k\delta t}$. Yet this is only an approximation as there is always a positive probability that the particle crosses the interface between $k\delta t$ and $(k+1)\delta t$. However, as long as $|X_{k\delta t}| \gg \sqrt{\delta t}$, this probability is exponentially small and may be neglected.

We are then concerned by setting up algorithms when $X_{k\delta t}$ belongs to an interval of length proportional to $\sqrt{\delta t}$ around 0.

Condition ($\mathcal{I}1$)**.** With $\Phi(x) = \int_0^x \mathrm{d}y/\sqrt{2D(y)}$, the stochastic process $Y_t = \Phi(X_t)$ is solution to the SDE with local time

$$Y_t = Y_0 + W_t + \theta L_t^0(Y),$$

where W is a Brownian motion, $L_t^0(Y)$ is the local time of Y at 0 and $\theta \in (-1,1)$ is a function of D^+, D^- and q. For example, with a divergence form operator $\nabla(D\nabla\cdot)$, $\theta = (\sqrt{D^+} - \sqrt{D^-})/(\sqrt{D^+} + \sqrt{D^-})$ while with a non-divergence form operator $D\triangle$, $\theta = (\sqrt{D^-} - \sqrt{D^+})/(\sqrt{D^+} + \sqrt{D^-})$.

The local time $L_t^0(Y)$ characterizes the time spend at 0 by the process: $L_t^0(Y) = \lim_{\epsilon\to 0}(2\epsilon)^{-1}\lambda(\{s \leq t; Y_s \in [-\epsilon, \epsilon]\})$, where λ is the Lebesgue measure. The paths

$t \mapsto L_t^0(Y)$ of this process are continuous and non-decreasing. They increase only on a set of measure 0 which is the closure of $\{t \geq 0; Y_t = 0\}$. These properties are a by-product of the irregularities of the paths of the Brownian motion.

The process Y is called a *Skew Brownian motion* [6]. Using its properties, several algorithms may be given. Also, its density has a simple form: $p(t, x, y) = \gamma(t, y - x) + \operatorname{sgn}(y)\theta\gamma(t, |x| + |y|)$, where $\gamma(t, x) = (2\pi t)^{1/2} \exp(-|y - x|^2/2t)$ is the Gaussian density.

In [8], we propose a simulation method in which $Y_{(k+1)\delta t}$ is exactly simulated when $Y_{k\delta t} = x$ is known using the expression of its density $p(\delta t, x, \cdot)$. Other algorithms, either based on probabilistic or analytic considerations, are also possible (See [8] for references).

These works justify the old heuristic that the interface acts like a permeable barrier. But due to the irregularities of the path, one has to look more closely to the properties of the process X or Y to give a sound meaning to this statement.

Although we present here some results specific to one-dimensional media, other algorithms have been proposed for multi-dimensional media with locally isotropic or orthotropic coefficients with a flat interface. In particular, in [7], we propose schemes with a better order of convergence than just moving the component of the process in the normal direction of the interface as in the one-dimensional case. For layered media, the scheme proposed in [5], which relies on some considerations of stochastic analysis, provides a simple and exact simulation technique.

Condition ($\mathcal{I}2$)**.** The interface condition ($\mathcal{I}2$) is seen as a semi-permeable barrier: the particle is reflected on the interface until it crosses it and starts afresh on the other side.

Using tools from stochastic analysis and the properties of the elastic Brownian motion which is linked to the Robin boundary conditions, we construct in [4] a diffusion process X associated to ($\star$) with the interface condition ($\mathcal{I}2$) by gluing together elastic Brownian motions. The time at which the particle passes for the first time to the other side of the interface is the smallest time at which the local time of the Brownian motion is greater than an independent exponential random variable of parameter λ when $D = 1/2$. We also provide a simple simulation algorithm.

Open problems. Many problems remain open regarding interface conditions, among them:

- The presence of a drift/convection term (See however [1]).
- The multi-dimensional case when the diffusivity tensor is not diagonal on each side of the interface.
- High contrasts ($D^+ \gg D^-$), where some techniques related to rare events simulations shall be used.

Acknowledgment. The body of work presented here has been initiated years ago and has been the subject to several collaborations. I then wish to thank M. Martinez, P. Étoré in addition to S. Maire and G. Pichot for works and discussions on interface condition ($\mathcal{I}1$) and J.-R. Li and D. Grebenkov for having suggested working on interface condition ($\mathcal{I}2$) and discussions about it.

References

[1] P. Étoré and M. Martinez. Exact Simulation of One-dimensional Stochastic Differential Equations involving the local time at zero of the unknown process (2011) arxiv:`1102.2565`

[2] M. Hairer and C. Manson. Periodic homogenization with an interface: the one-dimensional case. *Stoch. Proc. Appl.* **120**:8 (2010) 1589–1605.

[3] O. A. Ladyženskaja, V. Ja. Rivkind, and N. N. Ural'ceva. Solvability of diffraction problems in the classical sense, *Trudy Mat. Inst. Steklov.* **92** (1966) 116–146.

[4] A. Lejay. The snapping-out Brownian motion (2013). Preprint.

[5] A. Lejay. Simulation of a stochastic process in a discontinuous layered medium. *Electron. Commun. Probab.* **16** (2011) 764–774.

[6] A. Lejay. On the constructions of the skew Brownian motion. *Probab. Surv.* **3** (2006) 413–466.

[7] A. Lejay and S. Maire. New Monte Carlo schemes for simulating diffusions in discontinuous media. *J. Comput. Appl. Math.* **245** (2013) 97–116.

[8] A. Lejay and G. Pichot, Simulating diffusion processes in discontinuous media: a numerical scheme with constant time steps, *J. Comput. Phys.* **231**:21 (2012) 7299–7314.

[9] E. Sánchez-Palencia. *Non-Homogeneous Media and Vibration Theory*, Lecture Notes in Phys. **127** (1980), Springer.